

(NASA-CR-138306) NUCLEAR QUADRUPOLE
RESONANCE STUDIES IN SEMI-METALLIC
STRUCTURES Semiannual Status Report
(Grambling State Univ., La.) 32 p HC
\$4.75

N74-31023

Unclas
45718

CSCL 11D G3/18

DEPARTMENT OF
PHYSICS
GRAMBLING COLLEGE
Grambling, Louisiana

Third
Semi-Annual Status Report
on the project

NUCLEAR QUADRUPOLE RESONANCE STUDIES
IN SEMI-METALLIC STRUCTURES
(NGR-19-011-016)

by

A. Narasimha Murty
Department of Physics
Grambling State University

August 15, 1974

THIRD SEMI-ANNUAL STATUS REPORT

SUBMITTED TO:

NASA Scientific and Technical
Information Facility
Post Office Box 33
College Park, Maryland 20740

REFERENCE NUMBER:

NGR-19-011-016
Supplement No. I

INSTITUTION:

Grambling State University
Grambling, Louisiana 71245

TITLE:

Study of the Distribution of
Extra-Ionic Electrons in Semi-
Metallic Environments by
Nuclear Quadrupole Resonance
Techniques

PRINCIPAL INVESTIGATOR:

Dr. A. N. Murty, Professor
Department of Physics

DURATION:

Original Grant
Supplement No. I

One (1) Year
One (1) Year

SUM GRANTED BY NASA:

\$15,305 (1st Year)
\$17,494 (2nd Year)

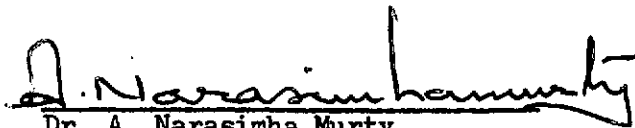
DATE:

(Project Started)
(1st Semi-Annual Report)
(2nd Semi-Annual Report)
(3rd Semi-Annual Report)

January 1, 1973
October 12, 1973
February 18, 1974
August 15, 1974

SIGNATURE:

Principal Investigator


Dr. A. Narasimha Murty
Department of Physics
Grambling State University
Grambling, Louisiana 71245

INTRODUCTION

This report describes the results of our studies in the Nuclear Quadrupole Resonance project at Grambling State University, sponsored by the National Aeronautics and Space Administration. The results are presented in two sections: A-experimental, and B-theoretical. Section A deals with an analysis of the NQR spectra of the tellurides of Antimony and Arsenic, and Section B presents numerical solutions for the secular equations of the quadrupole interaction energy.

A. Experimental:

Nuclear quadrupole resonance studies of the oxides, sulfides, and selenides of Arsenic and Antimony have been made by earlier investigators.¹⁻⁷ The tellurides of Arsenic and Antimony have been studied by us for the first time in this laboratory with a view to complete the data for the V and VI group compounds and examine the nature of bonding.

The chemicals As_2Te_3 and Sb_2Te_3 were obtained from Alfa Inorganics, Ventron Corporation, Beverley, Massachusetts. The samples were finely powdered and sifted through a 325 mesh sieve. The samples were very lossy when directly introduced in the R.F. coil of the oscillator. They were mixed with 325 mesh vycor glass powder, 50% by volume to reduce the R.F. losses.

The NQR spectra were observed on a Wilks servo controlled coherent super-regenerative NQR spectrometer. The frequency measurements were made by beating a standard signal generator (McGraw-Edison Model 80) with the NQR oscillator just before and after the observation of the resonance. Since the signal is repeated in a number of side bands, the resonance frequency is

Reproduced from
best available copy.



116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

116.7

114.5

114.5

34

MADE IN U.S.A.

MADE IN U.S.A.

taken as the centre of the envelop by interpolating between the two frequency markers. The marker frequencies were directly read from a GR 1192 Z counter-scaler unit connected to the standard signal generator. A representative signal pattern along with the markers is shown in Figure 1. Each measurement is repeated six times and the average value of frequency is used in estimating the coupling constant e^2Qq .

Results and Discussion:

The measured resonance frequency of As^{75} in Arsenic telluride (As_2Te_3) and the frequencies for the two isotopes of Antimony Sb^{121} , and Sb^{123} in Antimony telluride (Sb_2Te_3) are presented in Table I. All measurements were made at room temperature.

Since the spin of As^{75} is $3/2$, and only one isotope is present with natural abundance of 100%, in the absence of unequal crystalline environments; one resonance line is expected due to the transition between the energy levels $E_{3/2} \rightleftharpoons E_{1/2}$. The resonance frequency is given by⁵

$$\nu = 1/2 e^2Qq_{zz} (1 + \frac{\eta^2}{3})^{1/2} \quad - - - - - (1)$$

where Q is the nuclear quadrupole moment, q_{zz} the field gradient tensor component along the principal axis of symmetry and η the asymmetry parameter

$$\text{defined by } \eta = \frac{q_{xx} - q_{yy}}{q_{zz}} \quad - - - - - (2)$$

The nuclear quadrupole coupling constant e^2Qq given in Table I is obtained by doubling the NQR frequency assuming that η is very small. At present, no crystal structure data is available for As_2Te_3 to justify the assumption; but it may not be far from being correct since the metal atom in the homologues Sb_2Te_3 and Bi_2Te_3 are in highly symmetric environments.

TABLE I

COMPOUND	SPIN	NATURAL ABUNDANCE PERCENT	TRANSITION	FREQUENCY MHz	QUADRUPOLE COUPLING CONSTANT MHz	UNBALANCED P-ELECTRON U_p	
						EXPER.	CAL.
As_2Te_3 (As^{75})	$\frac{3}{2}$	100	$\frac{3}{2} \rightleftharpoons \frac{1}{2}$	115.9 ± 0.5	232 ± 1	0.386	---
Sb_2Te_3 (Sb^{121})	$\frac{5}{2}$	57	$\frac{3}{2} \rightleftharpoons \frac{1}{2}$	82.8 ± 0.2	552 ± 1	0.276	0.056
(Sb^{121})	$\frac{5}{2}$	57	$\frac{5}{2} \rightleftharpoons \frac{3}{2}$	165.3 ± 0.5	551 ± 2	0.276	0.056
(Sb^{123})	$\frac{7}{2}$	43	$\frac{3}{2} \rightleftharpoons \frac{1}{2}$	50.1 ± 0.2	701 ± 1	0.280	0.056

$$\text{Ratio } \frac{(e^2Qq)_{123}}{(e^2Qq)_{121}}$$

Present Estimate = 1.271

Literature Value⁵ = 1.274

The crystal structure of Sb_2Te_3 is⁸ rhombohedral. The corresponding hexagonal cell containing three molecules has the following unit cell dimensions. $A_0 = 4.25$ A.U. and $C_0 = 30.4$ A.U. This structure can be imagined as composed of layers of atoms along C axis following one another in the succession Te-Sb-Te-Te-Sb-Te-Te-. The immediate neighbor environment of the Antimony atoms is shown in Figure 2. Each Antimony atom (centre circle) is surrounded by 6 tellurium atoms. Three tellurium atoms (broken circles) are 1.69 A.U. above the plane of the paper at a distance of 2.98 A.U. from Sb, and three are 2.03 A.U. below the plane at a distance of 3.18 A.U. As such, the asymmetry parameter becomes zero and the quadrupole resonance frequencies can be directly expressed in terms of the quadrupole coupling constant e^2Qq_{zz} . Antimony has two isotopes: Sb^{121} and Sb^{123} with natural abundance of 57 and 43 percent respectively. For the isotope Sb^{121} having a spin of 5/2, two lines are expected with resonance frequencies given by⁵

$$\nu_1 = \frac{E_{3/2} - E_{1/2}}{h} = \frac{3}{20} e^2Qq_{zz} \left(1 + \frac{59}{54} \eta^2 - \dots\right) \quad (3)$$

$$\nu_2 = \frac{E_{5/2} - E_{3/2}}{h} = \frac{3}{10} e^2Qq_{zz} \left(1 - \frac{11}{54} \eta^2 + \dots\right) \quad (4)$$

The observed frequencies, and the coupling constants obtained by substituting $\eta = 0$ in the above equations are shown in Table I. For the isotope Sb^{123} , the spin is 7/2 and the three resonance frequencies are given by⁵

$$\nu_1 = \frac{E_{3/2} - E_{1/2}}{h} = \frac{1}{14} e^2Qq_{zz} \left(1 + \frac{109}{30} \eta^2 - \dots\right) \quad (5)$$

$$\nu_2 = \frac{E_{5/2} - E_{3/2}}{h} = \frac{1}{7} e^2Qq_{zz} \left(1 - \frac{17}{30} \eta^2 + \dots\right) \quad (6)$$

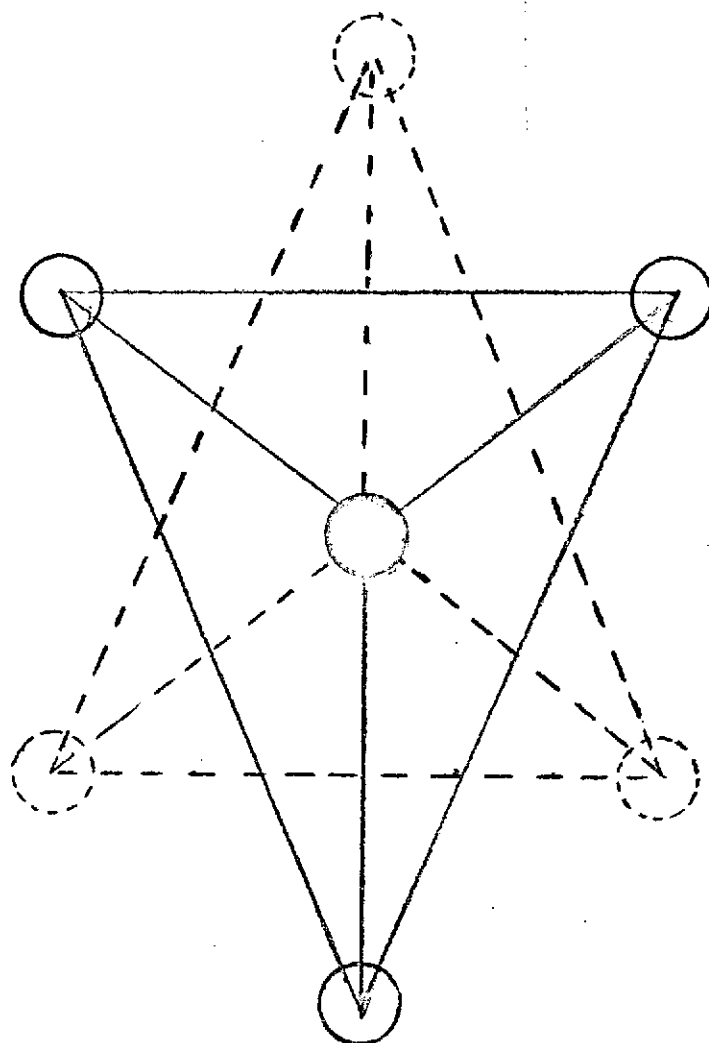


Figure 2: THE IMMEDIATE NEIGHBOR ENVIRONMENT IN ANTIMONY TELLURIDE

$$\nu_3 = \frac{E_{7/2} - E_{5/2}}{h} = \frac{3}{14} e^2 Qq_{zz} \left(1 - \frac{1}{10} \eta^2 - \dots\right) \quad (7)$$

Of the three expected lines only ν_1 could be observed. Even after annealing at 500°C for 24 hours, there appeared no change in the intensity of the lines. Presently, we are scanning the spectra at dry ice and liquid nitrogen temperatures.

An elementary analysis of the bond character on the basis of Townes and Dailey theory^{9,10} is instructive and interesting. The observed quadrupole coupling constant is related to the coupling constant due to a pure p-electron by

$$e^2 Qq_{\text{obs}} = u_p e^2 Qq_{\text{nlo}} \quad (8)$$

$$e^2 Qq_{\text{nlo}} = -2e^2 Qq_{\text{nll}} \quad (9)$$

The atomic coupling constants for As⁷⁵ ($e^2 Qq_{411} = 300$ MHz) and Sb¹²¹ ($e^2 Qq_{511} = 1000$ MHz) are taken from Townes and Schallow Table⁹. The values of u_p , the number of unbalanced p-electrons calculated from equation (8) are given in Table I as the experimental value. If double bond character and d-hybridization are neglected; treating that each Antimony atoms has s-p hybridized orbitals which form three covalent bonds with the tellurium atoms, and an unshared pair, u_p can be expressed as¹³

$$u_p = -3\alpha(1-3\beta + 4\beta(1+\epsilon)) \quad (10)$$

where α is the s-character of the bond determined by the inter-orbital angle θ as

$$\alpha = \cos \theta / (\cos \theta - 1) \quad - - - - - (11)$$

where β is the ionic character and ϵ the screening constant. For Sb_2Te_3 the inter-orbital angle $\text{Te} \hat{\text{Sb}} \text{Te}$ is about 91° giving a value of 1.7% for α - the s-character of the bond. The electronegativity difference Δ for Sb-Te is about 0.3, and β the ionic character is about 6% (vide pages 236, 237 in Ref. 9). The unbalanced p-electron value calculated in Table I is obtained from equation (10). On this basis, the valence electron contribution to the field gradient is only about 20%.

There are various factors to be considered to account for this large difference. First, there are considerable uncertainties in the value of atomic quadrupole coupling constants and the electronegativity difference $\Delta_{\text{Sb-Te}}$ values used in arriving at u_p calculated. The literature values for e^2Qq_{510} for Sb¹²¹ range perhaps anywhere from 734 MHz - 2000 MHz^{14,15} and the electronegativity difference $\Delta_{\text{Sb-Te}}$ ranges anywhere¹⁶⁻¹⁸ from 0.3 - 0.19. Secondly, u_p value is very sensitive to the bond angle especially when it is very close to 90° and the validity of application of Townes and Dailey¹⁰ theory to such cases may not be justifiable.

In addition to these uncertainties there is one important factor to be considered particularly in the case of inter-semi-metallic structures. The compounds As_2Te_3 and Sb_2Te_3 are electrically conducting with a specific resistance ρ in the range of 10^2 ohm cm. A simple measurement on a compacted column of the powder gives values $\rho_{\text{Sb}_2\text{Te}_3} = 212$ ohm cm and $\rho_{\text{As}_2\text{Te}_3} = 296$ ohm cm. This value falls in between that of a metal ($\rho_{\text{metal}} \sim 10^6$ ohm cm) and a semi-conductor ($\rho_{\text{semi-conductor}} \sim 10^6$ ohm cm). Earlier measurements on the nuclear quadrupole resonance spectra of Gallium¹⁹, Indium²⁰, and Anti-

mony²¹ indicate that the usual metallic model consisting of positive ions situated in a smooth electronic charge distribution of conduction electrons is inadequate to explain the observed results and that the spatial p-electrons may not be completely delocalized and should provide appreciable contribution to the field gradient at the site of the quadrupole nucleus. In the case of the tellurides of Arsenic and Antimony, we believe that the conduction electron contribution to the field gradient might be appreciable.

Other P-Block Elements Studied:

Since the tellurides of Antimony and Arsenic present an interesting situation where both the ionic character and s-hybridization are very small, but the coupling constants are large; we felt further examination of this feature in the tellurides of Indium and Gallium should lead to a better understanding.

Unfortunately, the sesqui selenides and tellurides of Indium and Gallium have a deficit cubic structure which becomes hexagonal at high temperature. It has not been possible to observe resonance in these samples even after annealing at 1000°C. But the mono-selenides and tellurides of Indium and Gallium have a favorable structure amenable to NQR studies. In these structures double layers of metal atoms succeed double layers of metalloid atoms. Presently, we are scanning the spectra of InSe and GaSe.

A thorough search was made in the frequency region 5-50 MHz to observe the resonance of pure Bismuth. Bismuth has similar rhombohedral structure as Arsenic and Antimony. Finite field gradient, almost the same as in Antimony is expected at the site of the Bismuth nuclei.²⁷ Our repeated searches both at room temperature and liquid nitrogen temperatures proved negative. Annealing the sample at 250°C also did not improve the situation.

In accordance with our proposed plan, we have investigated a number of Indium and Bismuth doped Antimony samples. The samples were prepared in the zone levelling unit developed in our laboratory.²⁸ In the first place, the Antimony NQR signals in pure Antimony were neither sharp nor strong at room temperature. The resonance signals observed in the doped samples with impurity concentrations in range of 0.5 - 2.0 percent by weight were considerably weak and broad. It has not been possible to make any quantitative measurements since our present frequency measurement method is accurate only up to 0.1 MHz. Presently, we are adding a spectrum analyzer unit to our existing spectrometer system. With this improved facility we hope to be able to arrive at more quantitative data.

B. Numerical Solutions for Pure Quadrupole Interaction Secular Equations:

Introduction:

The assignment of the nuclear quadrupole resonance spectra of nuclei ($I > 5/2$) in asymmetric environments ($\eta \geq 0.5$) presently involves graphical methods^{23,24} based on the numerical eigen value tables of Cohen.²² From these tables the experimenter should develop the relative frequency factors (eigen value differences) and the possible ratios for the various frequencies, and plot these ratios as a function of the asymmetry parameter. By a trial and error process, one can arrive at the proper experimental ratio points that fall on the calculated ratio curves forming a straight line perpendicular to the η -axis. The η value is interpolated from the intersection of this ordinate and η -axis, and the coupling constant from the corresponding frequency factor curve.

We have developed ready reference tables for the determination of η and e^2Qq from the observed NQR frequencies for values of η ranging from 0 - 1 in intervals of 0.01 for all values of $I = 5/2, 7/2$, and $9/2$. So far such data is available in the form of eigen values only from Cohen's tables²², for values of η from 0.1 to 1.0 in intervals of 0.1 for all values of $I = 5/2, 7/2$, and $9/2$; and from the tables of Livingston and Zeldes²⁵ for $I = 5/2$ with η ranging from 0 to 1 at intervals of 0.001. The latter is only for $I = 5/2$ and available in the Oak Ridge National Laboratory reports. Hence, the complete set of tables developed by us giving the frequency ratios and corresponding asymmetry parameters directly should be very convenient for the assignment of the NQR spectra.

Numerical Method:

The secular equations for pure quadrupole interaction energy^{23,26} are given in Table II.

Exact solutions of E can be obtained only for $I = 3/2$, and the transition frequency $\nu_{1/2}(3/2 \rightleftharpoons 1/2)$ is given by $\frac{E_{3/2} - E_{1/2}}{h} = \frac{e^2Qq}{2h} (1 + \eta^2/3)^{1/2}$. Since only one resonance line will be observed it is not possible to obtain both the asymmetry parameter η , and the quadrupole coupling constant e^2Qq separately unless one studies the zeeman spectra. For nuclei of spin values $I > 5/2$, there are two or more transition frequencies connecting the two unknowns η and e^2Qq and hence both can be obtained. But unfortunately it is not possible to obtain exact solutions in closed form as for $I = 3/2$, for the secular equations for spin values $I > 5/2$.

Bersohn²⁶ and Wang⁵ have obtained the solutions by a perturbation procedure in the form of an expansion series in powers of η^2 up to η^8 . These

TABLE II

<u>I</u>	<u>UNITS OF E</u>	<u>SECULAR EQUATION</u>	
$I = \frac{3}{2}$	$\frac{e^2 Q q}{12}$	$E^2 - 3\eta^2 - 9 = 0$	(1)
$I = \frac{5}{2}$	$\frac{e^2 Q q}{20}$	$E^3 - 7(3+\eta^2)E - 20(1-\eta^2) = 0$	(2)
$I = \frac{7}{2}$	$\frac{e^2 Q q}{28}$	$E^4 - 42(1+\eta^2/3)E^2 - 64(1-\eta^2)E + 105(1+\eta^2/3)^2 = 0$	(3)
$I = \frac{9}{2}$	$\frac{e^2 Q q}{24}$	$E^5 - 11(3+\eta^2)E^3 - 44(1-\eta^2)E^2 + \frac{44}{3}(3+\eta^2)^2E + 48(3+\eta^2)(1-\eta^2) = 0$	(4)

expressions are not valid for values of $\eta > 0.5$ and introduce significant errors²³ even for $\eta = 0.1$; for the lower transitions of high spin nuclei; such as the $3/2 \Rightarrow 1/2$ transitions of Bismuth and Indium compounds for which $I = 9/2$.

Using Newton Raphson²⁹ iteration method we have obtained numerical solutions to the secular equations. The computations were carried out on the IBM 360 computer at Louisiana Tech University, Ruston, Louisiana. The program involves obtaining successive values of energy for the secular equation starting from a trial value until the successive values are satisfactorily convergent. We have conveniently used Cohen's²² initial values as our starting eigen values (E_i).

The general iteration formula is given by:

$$E_{i+1} = E_i - \frac{F(E_i)}{F'(E_i)}$$

and the iteration process is continued until $E_{i+1} - E_i = 0.0001$. The iteration formulae used for obtaining eigen values for spin values $I = 5/2, 7/2$, and $9/2$ are given in Table III. The eigen values (E_i) obtained for all η values ranging from 0 - 1 at intervals of 0.01 are presented in the enclosed set of tables.

Explanation and Use of Tables:

The results are presented in three sets of tables for the three spin values $I = 5/2, 7/2$, and $9/2$. The $\left(\frac{2I+1}{2}\right)$ eigen values (E_m values, $m = 1/2, 3/2, 5/2, 7/2$, and $9/2$) for each spin value are given in multiples of $e^2 Qq$ as indicated in Table II, in successive columns corresponding to the value of the asymmetry parameter. Following these, the various frequency factor

TABLE III

$$I = \frac{5}{2}:$$

$$E_{i+1} = \frac{2E_i^3 + 20(1-\eta^2)}{3E_i^2 - 7(3+\eta^2)}$$

$$I = \frac{7}{2}:$$

$$E_{i+1} = \frac{3E_i^4 - 42\left(1+\frac{\eta^2}{3}\right)E_i^2 - 105\left(1+\frac{\eta^2}{3}\right)^2}{4E_i^3 - 84\left(1+\frac{\eta^2}{3}\right)E_i - 64(1-\eta^2)}$$

$$I = \frac{9}{2}:$$

$$E_{i+1} = \frac{4E_i^5 - 22(3+\eta^2)E_i^3 - 44(1-\eta^2)E_i^2 - 48(3+\eta^2)(1-\eta^2)}{5E_i^4 - 33(3+\eta^2)E_i^2 - 88(1-\eta^2)E_i + \frac{44}{3}(3+\eta^2)^2}$$

ratios are tabulated. For example E_{53}/E_{75} indicates the ratio of frequencies $\frac{\nu_2}{\nu_1} = \frac{E_{5/2} - E_{3/2}}{E_{3/2} - E_{1/2}}$ and E_{97}/E_{75} indicates the ratio $\frac{\nu_4}{\nu_3} = \frac{E_{9/2} - E_{7/2}}{E_{7/2} - E_{5/2}}$, etc.

With a tentative assignment for the observed NQR spectral lines one can easily verify whether the observed ratios of the assigned lines lie in the same row corresponding to a specific asymmetry parameter, in the table for that spin value. More accurate value of the asymmetry parameter up to a 3rd place can be obtained by interpolation. Now from the eigen value factors (E_m values) corresponding to the assigned asymmetry parameter the frequency factors (f) can be readily obtained; as the eigen value differences ($E_m - E_{m-1}$) for the energy levels representing the transition. The quadrupole coupling constant can be evaluated using this factor $f_{m(m-1)}$ and the observed resonance frequency $\nu_{m(m-1)}$ as:

$$I = 5/2 \quad e^2 Qq = \frac{20 h \nu_{m(m-1)}}{f_{m(m-1)}}$$

$$I = 7/2 \quad e^2 Qq = \frac{28 h \nu_{m(m-1)}}{f_{m(m-1)}}$$

$$I = 9/2 \quad e^2 Qq = \frac{24 h \nu_{m(m-1)}}{f_{m(m-1)}}$$

224

TABLES
OF
NUCLEAR QUADRUPOLE RESONANCE
FREQUENCY RATIOS AND ASSYMETRY PARAMETERS

$$I = 5/2$$

ASYMETRY	E5/2	E3/2	E1/2	E53/E31
0.0	5.00000	-1.00000	-4.00000	2.00000
0.01	5.00002	-0.99985	-4.00018	1.99974
0.02	5.00011	-0.99940	-4.00071	1.99896
0.03	5.00025	-0.99865	-4.00160	1.99767
0.04	5.00044	-0.99760	-4.00284	1.99586
0.05	5.00069	-0.99626	-4.00444	1.99355
0.06	5.00100	-0.99461	-4.00639	1.99072
0.07	5.00136	-0.99267	-4.00869	1.98740
0.08	5.00178	-0.99044	-4.01134	1.98359
0.09	5.00225	-0.98791	-4.01434	1.97929
0.10	5.00278	-0.98509	-4.01768	1.97451
0.11	5.00336	-0.98199	-4.02137	1.96926
0.12	5.00400	-0.97860	-4.02541	1.96356
0.13	5.00469	-0.97492	-4.02978	1.95741
0.14	5.00545	-0.97096	-4.03449	1.95082
0.15	5.00625	-0.96672	-4.03953	1.94382
0.16	5.00712	-0.96221	-4.04491	1.93640
0.17	5.00804	-0.95743	-4.05061	1.92858
0.18	5.00901	-0.95237	-4.05664	1.92038
0.19	5.01004	-0.94705	-4.06299	1.91181
0.20	5.01113	-0.94147	-4.06966	1.90289
0.21	5.01227	-0.93563	-4.07665	1.89362
0.22	5.01347	-0.92954	-4.08394	1.88403
0.23	5.01473	-0.92319	-4.09154	1.87413
0.24	5.01605	-0.91660	-4.09945	1.86394
0.25	5.01742	-0.90976	-4.10766	1.85346
0.26	5.01884	-0.90269	-4.11616	1.84272
0.27	5.02032	-0.89538	-4.12495	1.83173
0.28	5.02186	-0.88784	-4.13403	1.82050
0.29	5.02346	-0.88007	-4.14339	1.80906
0.30	5.02512	-0.87209	-4.15303	1.79741
0.31	5.02683	-0.86389	-4.16294	1.78557

$$I = 5/2$$

ASSYMETRY	E5/2	E3/2	E1/2	E53/E31
0.31	5.02683	-0.86389	-4.16294	1.78557
0.32	5.02859	-0.85547	-4.17313	1.77356
0.33	5.03042	-0.84685	-4.18357	1.76138
0.34	5.03230	-0.83802	-4.19428	1.74906
0.35	5.03424	-0.82899	-4.20525	1.73661
0.36	5.03624	-0.81977	-4.21647	1.72403
0.37	5.03830	-0.81036	-4.22794	1.71135
0.38	5.04041	-0.80076	-4.23965	1.69857
0.39	5.04258	-0.79099	-4.25160	1.68570
0.40	5.04481	-0.78103	-4.26378	1.67277
0.41	5.04710	-0.77091	-4.27620	1.65978
0.42	5.04945	-0.76061	-4.28884	1.64674
0.43	5.05185	-0.75015	-4.30170	1.63366
0.44	5.05431	-0.73954	-4.31478	1.62055
0.45	5.05684	-0.72876	-4.32808	1.60742
0.46	5.05942	-0.71784	-4.34158	1.59428
0.47	5.06206	-0.70677	-4.35529	1.58114
0.48	5.06476	-0.69556	-4.36921	1.56801
0.49	5.06752	-0.68421	-4.38331	1.55490
0.50	5.07034	-0.67272	-4.39762	1.54181
0.51	5.07322	-0.66111	-4.41211	1.52874
0.52	5.07616	-0.64937	-4.42679	1.51572
0.53	5.07915	-0.63750	-4.44166	1.50274
0.54	5.08222	-0.62552	-4.45670	1.48981
0.55	5.08533	-0.61343	-4.47191	1.47694
0.56	5.08851	-0.60122	-4.48730	1.46413
0.57	5.09175	-0.58890	-4.50286	1.45138
0.58	5.09506	-0.57648	-4.51858	1.43871
0.59	5.09842	-0.56396	-4.53446	1.42611
0.60	5.10184	-0.55134	-4.55051	1.41359

$$I = 5/2$$

ASYMTRY	E5/2	E3/2	E1/2	E53/E31
0.61	5.10533	-0.53863	-4.56670	1.40116
0.62	5.10888	-0.52583	-4.58305	1.38881
0.63	5.11249	-0.51295	-4.59955	1.37656
0.64	5.11616	-0.49998	-4.61619	1.36439
0.65	5.11990	-0.48692	-4.63298	1.35233
0.66	5.12369	-0.47379	-4.64990	1.34036
0.67	5.12756	-0.46059	-4.66697	1.32849
0.68	5.13148	-0.44732	-4.68416	1.31673
0.69	5.13546	-0.43397	-4.70149	1.30508
0.70	5.13951	-0.42057	-4.71895	1.29353
0.71	5.14363	-0.40709	-4.73653	1.28209
0.72	5.14780	-0.39356	-4.75424	1.27076
0.73	5.15204	-0.37997	-4.77207	1.25954
0.74	5.15634	-0.36633	-4.79002	1.24843
0.75	5.16071	-0.35264	-4.80808	1.23744
0.76	5.16515	-0.33889	-4.82626	1.22656
0.77	5.16964	-0.32510	-4.84455	1.21580
0.78	5.17421	-0.31127	-4.86294	1.20515
0.79	5.17883	-0.29739	-4.88145	1.19462
0.80	5.18353	-0.28347	-4.90006	1.18421
0.81	5.18829	-0.26951	-4.91878	1.17391
0.82	5.19311	-0.25552	-4.93759	1.16372
0.83	5.19800	-0.24150	-4.95651	1.15366
0.84	5.20296	-0.22745	-4.97552	1.14371
0.85	5.20798	-0.21336	-4.99463	1.13387
0.86	5.21308	-0.19926	-5.01383	1.12416
0.87	5.21823	-0.18512	-5.03312	1.11455
0.88	5.22346	-0.17096	-5.05250	1.10507
0.89	5.22875	-0.15679	-5.07196	1.09570
0.90	5.23411	-0.14259	-5.09153	1.08644

20A

$$I = 5/2$$

ASYMMETRY	E5/2	E3/2	E1/2	E53/E31
0.91	5.23954	-0.12838	-5.11116	1.07729
0.92	5.24504	-0.11415	-5.13089	1.06826
0.93	5.25060	-0.09991	-5.15069	1.05934
0.94	5.25624	-0.08566	-5.17058	1.05054
0.95	5.26194	-0.07140	-5.19054	1.04184
0.96	5.26771	-0.05713	-5.21059	1.03325
0.97	5.27355	-0.04285	-5.23070	1.02478
0.98	5.27947	-0.02857	-5.25089	1.01641
0.99	5.28545	-0.01429	-5.27116	1.00815
1.00	5.29150	-0.00000	-5.29149	1.00000

80
p.223
A

$$I = 7/2$$

ASYMMETRY	E7/2	E5/2	E3/2	E1/2	E75/E31	E53/E31	E75/E53
0.0	7.00000	1.00000	-3.00000	-5.00000	3.00000	2.00000	1.50000
0.01	7.00002	1.00008	-2.99970	-5.00040	2.99891	1.99918	1.50007
0.02	7.00009	1.00033	-2.99876	-5.00165	2.99555	1.99666	1.50028
0.03	7.00021	1.00075	-2.99722	-5.00374	2.98998	1.99249	1.50063
0.04	7.00038	1.00133	-2.99507	-5.00664	2.98226	1.98670	1.50111
0.05	7.00058	1.00208	-2.99230	-5.01036	2.97241	1.97932	1.50173
0.06	7.00084	1.00300	-2.98894	-5.01490	2.96048	1.97038	1.50249
0.07	7.00114	1.00408	-2.98498	-5.02024	2.94659	1.95998	1.50337
0.08	7.00149	1.00534	-2.98046	-5.02637	2.93081	1.94818	1.50438
0.09	7.00189	1.00676	-2.97536	-5.03328	2.91320	1.93502	1.50551
0.10	7.00234	1.00834	-2.96971	-5.04097	2.89388	1.92059	1.50677
0.11	7.00282	1.01010	-2.96352	-5.04940	2.87300	1.90501	1.50813
0.12	7.00336	1.01202	-2.95681	-5.05857	2.85063	1.88834	1.50960
0.13	7.00394	1.01411	-2.94959	-5.06846	2.82689	1.87066	1.51117
0.14	7.00458	1.01638	-2.94187	-5.07907	2.80190	1.85208	1.51284
0.15	7.00526	1.01881	-2.93369	-5.09037	2.77577	1.83267	1.51460
0.16	7.00598	1.02141	-2.92505	-5.10233	2.74864	1.81256	1.51644
0.17	7.00675	1.02418	-2.91597	-5.11495	2.72060	1.79180	1.51836
0.18	7.00757	1.02712	-2.90647	-5.12821	2.69178	1.77049	1.52036
0.19	7.00843	1.03023	-2.89657	-5.14209	2.66228	1.74872	1.52241
0.20	7.00934	1.03351	-2.88629	-5.15656	2.63220	1.72657	1.52452
0.21	7.01031	1.03697	-2.87564	-5.17163	2.60164	1.70411	1.52669
0.22	7.01131	1.04059	-2.86465	-5.18725	2.57070	1.68141	1.52890
0.23	7.01236	1.04440	-2.85334	-5.20342	2.53947	1.65855	1.53114
0.24	7.01347	1.04837	-2.84171	-5.22012	2.50803	1.63558	1.53341
0.25	7.01462	1.05252	-2.82980	-5.23733	2.47644	1.61258	1.53570
0.26	7.01581	1.05684	-2.81762	-5.25502	2.44480	1.58958	1.53801
0.27	7.01705	1.06134	-2.80518	-5.27320	2.41315	1.56665	1.54033
0.28	7.01834	1.06601	-2.79250	-5.29184	2.38156	1.54381	1.54265
0.29	7.01967	1.07086	-2.77961	-5.31092	2.35009	1.52114	1.54496
0.30	7.02106	1.07588	-2.76651	-5.33043	2.31878	1.49864	1.54726
0.31	7.02250	1.08109	-2.75322	-5.35036	2.28767	1.47636	1.54954
0.32	7.02397	1.08647	-2.73975	-5.37068	2.25681	1.45432	1.55179
0.33	7.02550	1.09203	-2.72613	-5.39139	2.22622	1.43256	1.55401

$$I = 7/2$$

ASYMMTRY	E7/2	E5/2	E3/2	E1/2	E75/E31	E53/E31	E75/E53
0.34	7.02708	1.09777	-2.71236	-5.41248	2.19594	1.41109	1.55620
0.35	7.02869	1.10369	-2.69846	-5.43392	2.16599	1.38994	1.55833
0.36	7.03036	1.10979	-2.68444	-5.45571	2.13641	1.36913	1.56042
0.37	7.03208	1.11607	-2.67032	-5.47783	2.10721	1.34866	1.56244
0.38	7.03385	1.12253	-2.65610	-5.50029	2.07839	1.32855	1.56441
0.39	7.03567	1.12918	-2.64180	-5.52304	2.04998	1.30880	1.56630
0.40	7.03753	1.13601	-2.62744	-5.54609	2.02200	1.28945	1.56812
0.41	7.03944	1.14302	-2.61301	-5.56945	1.99443	1.27046	1.56985
0.42	7.04140	1.15021	-2.59853	-5.59307	1.96731	1.25186	1.57151
0.43	7.04340	1.15759	-2.58402	-5.61697	1.94062	1.23366	1.57306
0.44	7.04546	1.16516	-2.56949	-5.64113	1.91439	1.21585	1.57453
0.45	7.04756	1.17291	-2.55493	-5.66554	1.88858	1.19842	1.57589
0.46	7.04972	1.18085	-2.54036	-5.69020	1.86323	1.18140	1.57714
0.47	7.05191	1.18897	-2.52580	-5.71508	1.83832	1.16476	1.57828
0.48	7.05417	1.19728	-2.51124	-5.74021	1.81385	1.14851	1.57930
0.49	7.05647	1.20578	-2.49669	-5.76555	1.78983	1.13265	1.58021
0.50	7.05882	1.21447	-2.48218	-5.79111	1.76623	1.11717	1.58099
0.51	7.06122	1.22335	-2.46769	-5.81687	1.74307	1.10207	1.58164
0.52	7.06366	1.23241	-2.45324	-5.84283	1.72034	1.08734	1.58215
0.53	7.06615	1.24167	-2.43883	-5.86898	1.69803	1.07298	1.58253
0.54	7.06870	1.25111	-2.42447	-5.89533	1.67613	1.05898	1.58277
0.55	7.07129	1.26074	-2.41018	-5.92185	1.65464	1.04535	1.58286
0.56	7.07394	1.27056	-2.39594	-5.94855	1.63355	1.03206	1.58281
0.57	7.07663	1.28058	-2.38178	-5.97542	1.61286	1.01912	1.58260
0.58	7.07938	1.29078	-2.36769	-6.00246	1.59256	1.00652	1.58224
0.59	7.08216	1.30118	-2.35368	-6.02966	1.57264	0.99426	1.58173
0.60	7.08501	1.31176	-2.33975	-6.05701	1.55309	0.98231	1.58105
0.61	7.08790	1.32254	-2.32592	-6.08452	1.53391	0.97070	1.58022
0.62	7.09085	1.33351	-2.31218	-6.11217	1.51509	0.95939	1.57922
0.63	7.09384	1.34466	-2.29853	-6.13996	1.49662	0.94840	1.57806
0.64	7.09688	1.35601	-2.28499	-6.16790	1.47850	0.93770	1.57673
0.65	7.09998	1.36755	-2.27156	-6.19597	1.46071	0.92730	1.57523
0.66	7.10313	1.37928	-2.25823	-6.22417	1.44325	0.91719	1.57356
0.67	7.10633	1.39120	-2.24502	-6.25250	1.42611	0.90736	1.57172

$$I = 7/2$$

ASSYMETRY	E7/2	E5/2	E3/2	E1/2	E75/E31	E53/E31	E75/E53
0.68	7.10958	1.40331	-2.23192	-6.28096	1.40929	0.89780	1.56971
0.69	7.11287	1.41560	-2.21895	-6.30952	1.39278	0.88852	1.56753
0.70	7.11622	1.42809	-2.20609	-6.33821	1.37656	0.87950	1.56517
0.71	7.11962	1.44077	-2.19337	-6.36702	1.36064	0.87073	1.56264
0.72	7.12308	1.45363	-2.18077	-6.39594	1.34501	0.86222	1.55994
0.73	7.12659	1.46668	-2.16830	-6.42496	1.32966	0.85395	1.55706
0.74	7.13015	1.47992	-2.15597	-6.45410	1.31458	0.84592	1.55401
0.75	7.13376	1.49335	-2.14377	-6.48334	1.29976	0.83813	1.55079
0.76	7.13743	1.50696	-2.13171	-6.51268	1.28521	0.83056	1.54740
0.77	7.14114	1.52076	-2.11979	-6.54211	1.27091	0.82322	1.54383
0.78	7.14491	1.53474	-2.10801	-6.57164	1.25686	0.81609	1.54010
0.79	7.14873	1.54890	-2.09637	-6.60126	1.24306	0.80918	1.53619
0.80	7.15260	1.56325	-2.08488	-6.63098	1.22948	0.80247	1.53212
0.81	7.15653	1.57777	-2.07353	-6.66078	1.21614	0.79597	1.52788
0.82	7.16052	1.59248	-2.06233	-6.69067	1.20303	0.78966	1.52348
0.83	7.16454	1.60737	-2.05128	-6.72064	1.19013	0.78354	1.51891
0.84	7.16864	1.62244	-2.04037	-6.75070	1.17745	0.77761	1.51419
0.85	7.17278	1.63768	-2.02962	-6.78084	1.16499	0.77187	1.50931
0.86	7.17698	1.65310	-2.01902	-6.81107	1.15272	0.76629	1.50427
0.87	7.18124	1.66870	-2.00857	-6.84136	1.14065	0.76090	1.49909
0.88	7.18554	1.68447	-1.99827	-6.87173	1.12878	0.75567	1.49374
0.89	7.18990	1.70041	-1.98812	-6.90218	1.11710	0.75061	1.48826
0.90	7.19432	1.71652	-1.97814	-6.93270	1.10561	0.74571	1.48263
0.91	7.19880	1.73280	-1.96830	-6.96329	1.09429	0.74096	1.47686
0.92	7.20332	1.74925	-1.95861	-6.99395	1.08316	0.73637	1.47095
0.93	7.20790	1.76586	-1.94908	-7.02467	1.07220	0.73192	1.46490
0.94	7.21254	1.78264	-1.93971	-7.05547	1.06140	0.72762	1.45873
0.95	7.21723	1.79958	-1.93049	-7.08633	1.05078	0.72347	1.45242
0.96	7.22199	1.81669	-1.92142	-7.11726	1.04031	0.71944	1.44600
0.97	7.22680	1.83395	-1.91251	-7.14824	1.03001	0.71556	1.43945
0.98	7.23166	1.85138	-1.90375	-7.17929	1.01985	0.71180	1.43279
0.99	7.23659	1.86895	-1.89514	-7.21041	1.00985	0.70817	1.42601
1.00	7.24158	1.88669	-1.88669	-7.24158	1.00000	0.70466	1.41912

$$I = 9/2$$

ASYMMETRY	E9/2	E7/2	E5/2	E3/2	E1/2
0.0	6.00000	2.00000	-1.00000	-3.00000	-4.00000
0.01	6.00001	2.00005	-0.99990	-2.99962	-4.00053
0.02	6.00005	2.00019	-0.99959	-2.99852	-4.00212
0.03	6.00012	2.00042	-0.99908	-2.99669	-4.00478
0.04	6.00023	2.00075	-0.99836	-2.99411	-4.00847
0.05	6.00036	2.00117	-0.99744	-2.99087	-4.01319
0.06	6.00051	2.00168	-0.99631	-2.98697	-4.01890
0.07	6.00070	2.00229	-0.99497	-2.98239	-4.02563
0.08	6.00091	2.00299	-0.99343	-2.97721	-4.03327
0.09	6.00116	2.00378	-0.99168	-2.97143	-4.04179
0.10	6.00143	2.00467	-0.98972	-2.96510	-4.05126
0.11	6.00173	2.00565	-0.98756	-2.95827	-4.06155
0.12	6.00206	2.00672	-0.98518	-2.95096	-4.07262
0.13	6.00241	2.00789	-0.98259	-2.94321	-4.08451
0.14	6.00280	2.00916	-0.97979	-2.93505	-4.09712
0.15	6.00322	2.01051	-0.97678	-2.92653	-4.11040
0.16	6.00366	2.01196	-0.97355	-2.91767	-4.12438
0.17	6.00413	2.01350	-0.97010	-2.90852	-4.13900
0.18	6.00463	2.01514	-0.96644	-2.89911	-4.15422
0.19	6.00516	2.01687	-0.96257	-2.88948	-4.16999
0.20	6.00573	2.01870	-0.95847	-2.87965	-4.18630
0.21	6.00631	2.02062	-0.95415	-2.86965	-4.20312
0.22	6.00693	2.02264	-0.94962	-2.85953	-4.22042
0.23	6.00757	2.02475	-0.94486	-2.84928	-4.23818
0.24	6.00824	2.02695	-0.93987	-2.83895	-4.25637
0.25	6.00894	2.02925	-0.93466	-2.82856	-4.27497
0.26	6.00967	2.03165	-0.92923	-2.81814	-4.29395
0.27	6.01044	2.03414	-0.92357	-2.80770	-4.31330
0.28	6.01122	2.03672	-0.91768	-2.79725	-4.33300
0.29	6.01205	2.03940	-0.91157	-2.78684	-4.35304
0.30	6.01290	2.04218	-0.90522	-2.77647	-4.37338
0.31	6.01377	2.04505	-0.89865	-2.76614	-4.39402
0.32	6.01468	2.04802	-0.89184	-2.75590	-4.41495
0.33	6.01561	2.05108	-0.88481	-2.74574	-4.43615

33
61
A

$$I = 9/2$$

ASYMMETRY	E97/E31	E75/E31	E53/E31	E97/E53	E75/E53	E97/E75
0.0	4.000	3.000	2.000	2.000	1.500	1.333
0.01	3.996	2.997	1.998	2.000	1.500	1.333
0.02	3.986	2.989	1.992	2.001	1.501	1.333
0.03	3.968	2.975	1.982	2.002	1.502	1.333
0.04	3.943	2.957	1.968	2.004	1.503	1.334
0.05	3.912	2.933	1.950	2.006	1.504	1.334
0.06	3.875	2.905	1.929	2.009	1.506	1.334
0.07	3.833	2.873	1.905	2.012	1.508	1.334
0.08	3.786	2.837	1.878	2.015	1.510	1.334
0.09	3.735	2.799	1.850	2.019	1.513	1.334
0.10	3.680	2.757	1.819	2.023	1.516	1.335
0.11	3.622	2.713	1.786	2.028	1.519	1.335
0.12	3.562	2.667	1.753	2.032	1.522	1.335
0.13	3.500	2.620	1.718	2.037	1.525	1.336
0.14	3.437	2.572	1.683	2.043	1.529	1.336
0.15	3.373	2.523	1.647	2.048	1.532	1.337
0.16	3.308	2.474	1.611	2.053	1.536	1.337
0.17	3.243	2.425	1.575	2.059	1.539	1.338
0.18	3.179	2.376	1.540	2.064	1.543	1.338
0.19	3.115	2.327	1.505	2.070	1.546	1.339
0.20	3.051	2.278	1.470	2.075	1.550	1.339
0.21	2.989	2.231	1.436	2.081	1.553	1.340
0.22	2.928	2.184	1.403	2.086	1.556	1.340
0.23	2.868	2.138	1.371	2.091	1.559	1.341
0.24	2.809	2.093	1.340	2.096	1.562	1.342
0.25	2.751	2.049	1.309	2.101	1.565	1.343
0.26	2.695	2.006	1.280	2.106	1.568	1.344
0.27	2.641	1.964	1.251	2.110	1.570	1.344
0.28	2.588	1.924	1.224	2.115	1.572	1.345
0.29	2.536	1.884	1.197	2.118	1.574	1.346
0.30	2.486	1.846	1.172	2.122	1.575	1.347
0.31	2.438	1.808	1.147	2.125	1.576	1.348
0.32	2.391	1.772	1.124	2.128	1.577	1.349
0.33	2.345	1.737	1.101	2.130	1.578	1.350

$$I = 9/2$$

ASYMMETRY	$E9/2$	$E7/2$	$E5/2$	$E3/2$	$E1/2$
0.34	6.01657	2.05424	-0.87754	-2.73568	-4.45760
0.35	6.01757	2.05750	-0.87004	-2.72573	-4.47929
0.36	6.01859	2.06085	-0.86231	-2.71590	-4.50122
0.37	6.01964	2.06430	-0.85435	-2.70622	-4.52337
0.38	6.02071	2.06785	-0.84616	-2.69667	-4.54574
0.39	6.02183	2.07150	-0.83773	-2.68728	-4.56831
0.40	6.02297	2.07524	-0.82908	-2.67805	-4.59107
0.41	6.02413	2.07908	-0.82020	-2.66899	-4.61402
0.42	6.02533	2.08302	-0.81109	-2.66011	-4.63715
0.43	6.02656	2.08705	-0.80175	-2.65141	-4.66046
0.44	6.02782	2.09119	-0.79219	-2.64290	-4.68391
0.45	6.02911	2.09542	-0.78240	-2.63458	-4.70754
0.46	6.03042	2.09976	-0.77239	-2.62647	-4.73131
0.47	6.03177	2.10419	-0.76217	-2.61856	-4.75524
0.48	6.03314	2.10872	-0.75172	-2.61085	-4.77929
0.49	6.03455	2.11335	-0.74105	-2.60336	-4.80349
0.50	6.03598	2.11809	-0.73017	-2.59608	-4.82782
0.51	6.03745	2.12292	-0.71908	-2.58902	-4.85227
0.52	6.03894	2.12786	-0.70778	-2.58218	-4.87684
0.53	6.04047	2.13289	-0.69628	-2.57555	-4.90153
0.54	6.04203	2.13803	-0.68457	-2.56915	-4.92634
0.55	6.04360	2.14327	-0.67266	-2.56297	-4.95125
0.56	6.04523	2.14862	-0.66056	-2.55701	-4.97627
0.57	6.04687	2.15406	-0.64826	-2.55128	-5.00139
0.58	6.04854	2.15961	-0.63578	-2.54576	-5.02661
0.59	6.05025	2.16526	-0.62311	-2.54048	-5.05193
0.60	6.05199	2.17102	-0.61026	-2.53541	-5.07734
0.61	6.05375	2.17688	-0.59723	-2.53056	-5.10283
0.62	6.05555	2.18285	-0.58403	-2.52594	-5.12843
0.63	6.05738	2.18892	-0.57067	-2.52153	-5.15410
0.64	6.05923	2.19509	-0.55713	-2.51735	-5.17986
0.65	6.06113	2.20138	-0.54344	-2.51338	-5.20568
0.66	6.06305	2.20777	-0.52960	-2.50962	-5.23160
0.67	6.06500	2.21426	-0.51560	-2.50608	-5.25758

223

$$I = 9/2$$

ASYM.LTRY	E97/E31	E75/E31	E53/E31	E97/E53	E75/E53	E97/E75
0.34	2.301	1.703	1.079	2.132	1.578	1.352
0.35	2.258	1.669	1.058	2.134	1.578	1.353
0.36	2.217	1.637	1.038	2.135	1.577	1.354
0.37	2.177	1.606	1.019	2.136	1.576	1.355
0.38	2.138	1.576	1.001	2.136	1.575	1.357
0.39	2.100	1.547	0.983	2.136	1.573	1.358
0.40	2.064	1.518	0.967	2.135	1.571	1.359
0.41	2.028	1.491	0.951	2.134	1.568	1.361
0.42	1.994	1.464	0.935	2.132	1.565	1.362
0.43	1.961	1.438	0.921	2.130	1.562	1.364
0.44	1.929	1.413	0.907	2.127	1.558	1.365
0.45	1.898	1.388	0.893	2.124	1.554	1.367
0.46	1.867	1.365	0.881	2.120	1.549	1.369
0.47	1.838	1.342	0.869	2.116	1.544	1.370
0.48	1.810	1.319	0.857	2.111	1.539	1.372
0.49	1.782	1.297	0.846	2.106	1.533	1.374
0.50	1.756	1.276	0.836	2.100	1.526	1.376
0.51	1.730	1.256	0.826	2.093	1.520	1.377
0.52	1.704	1.236	0.817	2.087	1.513	1.379
0.53	1.680	1.216	0.808	2.079	1.505	1.381
0.54	1.656	1.197	0.800	2.072	1.498	1.383
0.55	1.633	1.179	0.791	2.063	1.490	1.385
0.56	1.611	1.161	0.784	2.055	1.481	1.387
0.57	1.589	1.144	0.777	2.046	1.473	1.389
0.58	1.568	1.127	0.770	2.036	1.464	1.391
0.59	1.547	1.110	0.763	2.026	1.454	1.393
0.60	1.527	1.094	0.757	2.016	1.445	1.395
0.61	1.507	1.078	0.752	2.005	1.435	1.398
0.62	1.488	1.063	0.746	1.994	1.425	1.400
0.63	1.469	1.048	0.741	1.983	1.415	1.402
0.64	1.451	1.034	0.736	1.971	1.404	1.404
0.65	1.434	1.020	0.732	1.959	1.393	1.406
0.66	1.416	1.006	0.727	1.947	1.382	1.408
0.67	1.400	0.992	0.723	1.935	1.371	1.411

0.34
0.35
0.36
0.37
0.38
0.39
0.40
0.41
0.42
0.43
0.44
0.45
0.46
0.47
0.48
0.49
0.50
0.51
0.52
0.53
0.54
0.55
0.56
0.57
0.58
0.59
0.60
0.61
0.62
0.63
0.64
0.65
0.66
0.67

$$I = 9/2$$

	ASSYMETRY	E9/2	E7/2	E5/2	E3/2	E1/2
	0.68	6.06698	2.22087	-0.50146	-2.50274	-5.28364
	0.69	6.06900	2.22758	-0.48717	-2.49962	-5.30978
	0.70	6.07104	2.23440	-0.47275	-2.49670	-5.33599
	0.71	6.07312	2.24133	-0.45820	-2.49399	-5.36226
	0.72	6.07523	2.24836	-0.44352	-2.49148	-5.38859
	0.73	6.07736	2.25551	-0.42872	-2.48917	-5.41500
	0.74	6.07955	2.26277	-0.41380	-2.48705	-5.44147
	0.75	6.08174	2.27014	-0.39877	-2.48513	-5.46800
	0.76	6.08397	2.27762	-0.38363	-2.48340	-5.49459
	0.77	6.08624	2.28521	-0.36838	-2.48185	-5.52123
	0.78	6.08854	2.29292	-0.35304	-2.48050	-5.54791
	0.79	6.09087	2.30074	-0.33761	-2.47932	-5.57468
	0.80	6.09323	2.30867	-0.32209	-2.47833	-5.60149
	0.81	6.09563	2.31672	-0.30648	-2.47751	-5.62835
	0.82	6.09805	2.32487	-0.29080	-2.47687	-5.65527
	0.83	6.10051	2.33315	-0.27504	-2.47640	-5.68223
	0.84	6.10301	2.34154	-0.25921	-2.47610	-5.70924
	0.85	6.10553	2.35005	-0.24331	-2.47596	-5.73631
	0.86	6.10810	2.35867	-0.22736	-2.47598	-5.76341
	0.87	6.11067	2.36741	-0.21135	-2.47617	-5.79057
	0.88	6.11330	2.37627	-0.19528	-2.47651	-5.81777
	0.89	6.11595	2.38524	-0.17917	-2.47701	-5.84503
	0.90	6.11864	2.39434	-0.16302	-2.47766	-5.87230
	0.91	6.12136	2.40355	-0.14682	-2.47846	-5.89964
	0.92	6.12412	2.41289	-0.13060	-2.47941	-5.92700
	0.93	6.12691	2.42234	-0.11434	-2.48049	-5.95442
	0.94	6.12972	2.43191	-0.09805	-2.48172	-5.98187
	0.95	6.13258	2.44161	-0.08174	-2.48309	-6.00936
	0.96	6.13547	2.45143	-0.06542	-2.48460	-6.03689
	0.97	6.13840	2.46137	-0.04908	-2.48623	-6.06446
	0.98	6.14136	2.47143	-0.03272	-2.48801	-6.09206
	0.99	6.14435	2.48162	-0.01636	-2.48991	-6.11970
	1.00	6.14737	2.49193	-0.00000	-2.49193	-6.14737

$$I = 9/2$$

ASSYMETRY	E97/E31	E75/E31	E53/E31	E97/E53	E75/E53	E97/E75
0.68	1.383	0.979	0.720	1.922	1.360	1.413
0.69	1.367	0.966	0.716	1.909	1.349	1.415
0.70	1.351	0.953	0.713	1.896	1.338	1.417
0.71	1.336	0.941	0.710	1.882	1.326	1.419
0.72	1.321	0.929	0.707	1.869	1.314	1.422
0.73	1.306	0.917	0.704	1.855	1.303	1.424
0.74	1.292	0.906	0.702	1.841	1.291	1.426
0.75	1.278	0.895	0.699	1.827	1.279	1.428
0.76	1.264	0.884	0.697	1.813	1.267	1.430
0.77	1.251	0.873	0.695	1.798	1.256	1.432
0.78	1.237	0.863	0.694	1.784	1.244	1.434
0.79	1.224	0.852	0.692	1.770	1.232	1.437
0.80	1.212	0.842	0.690	1.755	1.220	1.439
0.81	1.199	0.833	0.689	1.741	1.208	1.441
0.82	1.187	0.823	0.688	1.726	1.197	1.443
0.83	1.175	0.814	0.687	1.711	1.185	1.444
0.84	1.163	0.804	0.686	1.697	1.173	1.446
0.85	1.152	0.795	0.685	1.682	1.162	1.448
0.86	1.141	0.787	0.684	1.667	1.150	1.450
0.87	1.129	0.778	0.683	1.653	1.139	1.452
0.88	1.118	0.770	0.683	1.638	1.127	1.453
0.89	1.108	0.761	0.682	1.624	1.116	1.455
0.90	1.097	0.753	0.682	1.609	1.105	1.456
0.91	1.087	0.745	0.682	1.595	1.094	1.458
0.92	1.076	0.738	0.681	1.580	1.083	1.459
0.93	1.066	0.730	0.681	1.566	1.072	1.460
0.94	1.056	0.723	0.681	1.551	1.061	1.462
0.95	1.047	0.716	0.681	1.537	1.051	1.463
0.96	1.037	0.709	0.681	1.523	1.040	1.464
0.97	1.028	0.702	0.681	1.509	1.030	1.465
0.98	1.018	0.695	0.681	1.495	1.020	1.466
0.99	1.009	0.688	0.681	1.481	1.010	1.466
1.00	1.000	0.682	0.682	1.467	1.000	1.467

REFERENCES

1. Bray, P.J., G.O. O'Keefe and R.G. Barnes, J. Chem. Phys., 25, 792 (1956).
2. Crane, L., R. Anderson and H.G. Robinson, Bull. Amer. Chem. Soc. Ser. II, 4, 11 (1959).
3. Penkov, I.N. and I.A. Saffin, Tables of NQR Frequencies; I.P. Biryukov et al, Israel Program for Scientific Translations Jerusalem (1969).
4. Barnes, R.G. and P.J. Bray, J. Chem. Phys., 23, 1177 (1955).
5. Wang, T.C., Phys. Rev., 99, 566 (1955).
6. Chiba, T.J., Phys. Soc. Japan, 13, 860 (1958).
7. Penkov, I.N. and I.A. Saffin, Danssr, 153, 692 (1963).
8. Wyckoff, R.W.G., "Structures of Crystals", 2, 30 (1960); John Wiley and Sons: New York.
9. Townes, C.H. and A.L. Schallow, "Microwave Spectroscopy" (1955); McGraw-Hill Book Company: New York.
10. Townes, C.H. and B.P. Dailey, J. Chem. Phys., 17, 782 (1949); 20, 35 (1952); 23, 118 (1955).
11. King, J.G. and V. Jaccarino, Phys. Rev., 94, 1610 (1954).
12. Ramsey, N.F., "Nuclear Moments" (1953); John Wiley and Sons: New York.
13. Gordy, W., W.V. Smith and R.F. Trambarulo, "Microwave Spectroscopy" (1953); John Wiley and Sons: New York.
14. Shizuko Ogawa, J. Phys. Soc. Japan, 13, 618 (1958).
15. Lucken, E.A.C., "Nuclear Quadrupole Coupling Constants" (1969), p. 276; Academic Press: New York.
16. Pauling, L., Nature of the Chemical Bond; Cornell University Press: Ithaca, New York (1960).
17. Huggins, M.L., J. Amer. Chem. Soc., 75, 4123 (1953).
18. Royer, D.J., "Bonding Theory" (1968); McGraw-Hill Book Co.: New York.
19. Knight, W.D., R.R. Hewitt and M. Pomerantz, Phys. Rev., 104, 271 (1956).

20. Simmons, W.W., and C.P. Slichter, Phys. Rev., 121, 1580 (1961).
21. Hewitt, R.R. and B.F. Williams, Phys. Rev., 129, 1188 (1963).
22. Cohen, M.H., Phys. Rev., 96, 1278 (1954).
23. Robinson, H.G., Phys. Rev., 100, 1731 (1955).
24. Swiger, E.D., P.J. Green, et al, J. Phys. Chem., 69, 949 (1965).
25. Livingston, R. and H. Zeldes, Tables of Eigen Values for Pure Quadrupole Spectra, Spin 5/2; Oak Ridge National Laboratory Report, ORNL-1913 (1955).
26. Bersohn, R., J. Chem. Phys., 20, 1505 (1952).
27. Taylor, T.T. and E.H. Hygh, Phys. Rev., 129, 1193 (1963).
28. A. Narasimhamurty, Second Semi-Annual Status Report (1974), NASA Scientific and Technical Information Facility; College Park, MD.
29. Hildebrand, F.B., (1974) "Introduction to Numerical Analysis"; McGraw-Hill Book Company: New York.